Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.01e-05 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.50e-01

Confidence level: 5.60e-01

Nearest Neighbors from the Training Set

Image not found
Naled
Measured: 2.85e-05
Predicted: 5.68e-04

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3,4,5,6-Tetrachloroguaiacol
Measured: 8.48e-07
Predicted: 1.70e-04

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Oxazole
Measured: 9.75e-05
Predicted: 99.5

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Ethirimol
Measured: 2.40e-07
Predicted: 1.10e-06

Image not found
Hymexazol
Measured: 3.20e-04
Predicted: 1.02e-02